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Physics-based hydrologic response simulation: platinum bridge, 1958 Edsel, or useful tool

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> **The aim of a model is, of course, precisely not to reproduce reality in all its complexity. It is rather to capture in a vivid, often formal, way what is essential to understanding some aspect of its structure or behavior. . .. We select, for inclusion in our model, those features of reality that we consider to be essential to our purpose . . . the ultimate criteria, being based on intentions and purposes as they must be, are finally determined by the individual, that is, human, modeler.**
>
> **Joseph Weizenbaum (1976)**

There are Lots (and Lots) of Rainfall-Runoff Models

Clarke (1973) generalizes a mathematical rainfall-runoff model by

$$q_t = f(p_{t-1}, p_{t-2}, \ldots; q_{t-1}, q_{t-2}, \ldots; a_1, a_2, \ldots) + \xi_t \qquad (1)$$

where p_t are the input variables, q_t are the output variables, a_n are the system parameters, ξ_t is the residual error, and f is the functional form of the model. Encoded in this relationship is a fundamental distinction between model elements (i.e. variables change with time, parameters remain constant). The functional form of the relationship can be conceptual or empirical; the input and output variables, as well as the system parameters and residual error, can be either stochastic or deterministic. A model is stochastic if any of the variables are described by a probability distribution; it is deterministic if all the variables are (viewed as) free from random variations. Models are conceptual if their functional form is derived from consideration of physical processes, and empirical if not. Clarke (1973) categorizes mathematical models as stochastic-conceptual, stochastic-empirical, deterministic-conceptual, or deterministic-empirical.

In the last half-century there have been hundreds (if not thousands) of hydrologic-response models, each with their own attributes and shortcomings, developed by researchers, students, and consultants, covering the entire spectrum of Clarke's classification. It is important to recognize that not all of these models were created equally. The relatively simple empirical models, whose system parameters cannot (most often) be measured in the field, perform successfully only within a calibrated range. Many conceptual models have been developed around a single process (e.g. the Horton mechanism). A typical example of the misuse of the single-process

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Table I. Characteristics[a] of selected physically based and quasi-physically based models of water flow and solute transport that have been and/or are currently being employed for concept-development purposes related to near-surface hydrologic-response processes (modified from Loague *et al.* (2004))

Primary reference	Subsurface	Surface		Coupling
		Overland	Open-channel	
Freeze (1971, 1972a,b)	3D-F, U/S, N/R	na	1D-F, N/DW	SQ
Smith and Woolhiser (1971)	1D-F, U, N/R	1D-F, N/K	1D-F, N/K	SQ
Engman and Rogowski (1974)	1D-F, U, A	1D-F, N/K	1D-F, N/K	SQ
Beven (1977)	2D-F, U/S, N/R	na	1D-F, N/DW	SQ
Beven and Kirkby (1979)	1D-F, U/S, E	1D-F, E	1D-F, E	SQ
Ross *et al.* (1979)	1D-F, U, E	1D-F, N/K	1D-F, E	SQ
Alley *et al.* (1980)	1D-F, U, E	1D-F, N/K	1D-F, N/K	SQ
Akan and Yen (1981a,b)	2D-F, U/S, N/R	1D-F, N/DW	1D-F, N/DW	SQ
Leavesley *et al.* (1983)	1D-F, U/S, E	1D-F, N/K	1D-F, N/K	SQ
Smith and Hebbert (1983)	2D-F, U/S, A	1D-F, N/K	1D-F, N/K	SQ
Abbott *et al.* (1986)	1D-F/T, U, N/RT; 2D-F/T, S, N/GT	2D-F, N/DW	1D-F, N/DW	SQ
Beven *et al.* (1987)	2D-F, U/S, N/R	1D-F, N/K	1D-F, N/K	SQ
Binley *et al.* (1989)	3D-F, U/S, N/R	1D-F, E	1D-F, E	SQ
Woolhiser *et al.* (1990)	1D-F, U, A	1D-F, N/K	1D-F, N/K	SQ
Govindaraju and Kavvas (1991)	2D-F, U/S, N/R	1D-F, N/DW	1D-F, N/DW	SQ
Moore and Grayson (1991)	1D-F, U, E	1D-F, E	1D-F, E	SQ
Wigmosta *et al.* (1994)	1D-F, U, E; 3D-F, S, E	1D-F, E	1D-F, E	SQ
Wigmosta and Burges (1997)	2D-F, U/S, A	1D-F, E	1D-F, E	SQ
VanderKwaak (1999)	3D-F/T, U/S, N/RT	2D-F/T, N/DWT	2D-F/T, N/DWT	FO
Morita and Yen (2000, 2002)	3D-F, U/S, N/R	2D-F, N/I	2D-F, N/I	SQ

[a] 1D, 2D, 3D (dimensions); F/T [flow (water)/(solute) transport]; U (unsaturated); S (saturated); U/S (unsaturated/saturated); N (numerical solution); A (analytical solution); E (empirical solution); R (Richards); RT (Richards and advection dispersion); G (groundwater); GT (groundwater and advection dispersion); DW (dynamic wave); DWT (dynamic wave and solute transport); I (noninertial wave); K (kinematic wave); SQ (sequential); FO (first order).

approach is the rainfall-runoff simulations reported by Loague and Freeze (1985), where a Horton-type model was employed (prior to visiting the site) to simulate hydrologic response for a small rangeland catchment before it was known that the Dunne mechanism can be important (see VanderKwaak and Loague (2001)). Table I shows an abbreviated summary of the evolution of deterministic-conceptual hydrologic-response models. Perusal of the 20 entries in Table I clearly shows, as previously stated, that models are not all created equally. It is also clear that not all models described as physically based are based on physics. Depending upon the purpose of the simulation, it can be essential to get as much of the physics correct as possible. For example, estimating the spatial and temporal variability of surface water depths and velocities (e.g. to drive an erosion model) or subsurface pore pressures (e.g. to drive a slope stability model) requires a conceptual model.

Early on, researchers assumed that deterministic-conceptual models, tested with exhaustive plot-scale data sets, could be employed (albeit with much more information needed) to simulate process-based hydrologic response at larger scales. This assumption was grounded in the fact that plots make up hillslopes, hillslopes make up catchments, and catchments make up watersheds. The fact is, however, related to physics-based near-surface hydrologic response simulation, that no existing catchment-scale data set has allowed (with high levels of confidence in both space and time) for a complete characterization of the boundary-value problem (BVP) or a rigorous evaluation of model performance. Paradoxically, detailed instrumentation and monitoring, when invasive, can modify system response.

> For a good mathematical model it is not enough to work well. It must work well for the right reasons.
>
> Vit Klemes (1986)

Better to be Wrong for the Right Reason Than Right for the Wrong Reason

Klemes (1997) wrote

> For hydrology as a science, the invasion of mathematical modeling was nothing short of a disaster. It has retarded rather than advanced the development of hydrology because, with very few exceptions, it focused all efforts on polishing the mathematical and computational aspects of methods and techniques, leaving the understanding of the substance at the 1930s level, where it had been brought by the old guard of professionals like Hazen, Sherman, Horton, Theis, to name a few.

The dismal picture painted by Klemes is food for thought. However, the more recent contributions of Al Freeze, Tom Dunne, Bill Dietrich, and Keith Beven (to name only a few of the principal players) have, without question, improved our understanding of near-surface processes and hydrologic response. The ongoing advances in quantitative hydrology are the result of both field study and simulation, which, as recognized by Robert E. Horton, are not mutually exclusive endeavors.

Freeze and Harlan (1969) proposed a blueprint for a distributed physically based hydrologic model, based upon numerical solution to the coupled partial differential equations that describe water movement at the surface and in the unsaturated and saturated subsurface. The development of Freeze's hydrologic-response model is now part of the classic literature in hillslope hydrology (Freeze, 1971, 1972a,b). It should be pointed out that the Freeze model simulated subsurface unsaturated–saturated fluid flow loosely coupled to open channel flow, but did not simulate overland flow (see Table I). Snyder (1973), commenting on Freeze's model, wrote

> The steps in classical scientific method might be personalized by the statement, I observed, I measured, I analyzed, I hypothesized. Sole reliance on computer simulation contains dangerous elements of a philosophy based on the premise, I constructed, I computed; therefore it is.

Obviously, sole reliance on computer modelling is not a wise tack for predicting hydrologic response (see Freeze's (1973) reply to the Snyder's comments). The problem, as already mentioned, is that the data do not exist to validate rigorously uncalibrated deterministic-conceptual models at any scale.

The Freeze and Harlan blueprint has recently come under scrutiny again (Beven, 2002a; Reggiani and Schellekens, 2003), due (in part) to the *equifinality* (Beven, 1993, 1996a,b, 2001a, 2004a; Brazier *et al*., 2000; Savenije, 2001) in scale-dependent model representations. Equifinality, in the context of deterministic-conceptual simulation, refers to more than one parameter set providing an equally good representation of overall hydrologic response. Savenije (2001) writes

> Although we can consider equifinality as a nuisance since it implies that looking for more understanding through detailed distributed modelling is a dead-end track, it also offers an opening to the revival of larger-scale hydrological laws.

Obviously, one should consider the intended use of a distributed model before characterizing the approach as a dead-end track (i.e. large scales are not always the focus). It is important to remember that the space of possible parameter values (and their combinations), which are not independent, can be constrained in a physics-based model. Without the physics, there are no such constraints, and any combination is valid.

There is now considerable literature focused on the nuances and problems associated with distributed hydrologic modelling (e.g. Beven, 1989, 1993, 1996a,b, 2000a,b, 2001b,c, 2002a,b; Beven and Binley, 1992; Woolhiser, 1996; Beven and Freer, 2001; Singh and Woolhiser, 2002). Some of the challenges in developing a physics-based hydrologic-response model are: (i) disparate time frames between the surface and subsurface flow regimes; (ii) strong nonlinearities in the governing equations; (iii) contrasting spatial discretization requirements; (iv) large unstructured grids; and (v) the spatial and temporal variability of the input parameters. Some of the challenges in the application of physics-based models are: (i) definition and resolution of surface topography; (ii) spatial and temporal variability of variables, parameters, and boundary conditions; (iii) upscaling (e.g. point measurements to element areas); (iv) preferential flow (e.g. macropores); and (v) process representation (e.g. use of Richards' equation for dual continuums). In our opinion, none of the development or application challenges listed here should result in an abandonment of the Freeze and Harlan blueprint.

The Integrated Hydrology Model (I*n*HM) is an example of a physics-based model that was developed (VanderKwaak, 1999) in the spirit of the Freeze and Harlan blueprint. I*n*HM was designed to estimate quantitatively, in a fully coupled approach, three-dimensional (3D) variably saturated flow and solute transport in porous media, 3D variably saturated flow and transport in macropores, and two-dimensional (2D) flow and transport over the surface and in open channels. The important and innovative characteristics of I*n*HM include: (i) adaptive temporal weighting and time stepping; (ii) robust and efficient iterative sparse-matrix solution methods with the solution precision and mass-balance error stipulated by convergence tolerances; (iii) solution of one system of discrete equations with spatially variable properties and boundary conditions that requires no iteration between separate models or model components and no artificial boundary conditions; (iv) allowing discontinuity of pressure across the subsurface–surface interface; and (v) no *a priori* assumption of a specific streamflow generation mechanism (i.e. Horton overland flow, Dunne overland flow, subsurface stormflow, groundwater). One of the goals associated with the development of I*n*HM was to establish a rigorous numerical framework onto which researchers could build and investigate different process conceptualizations. I*n*HM's first-order coupling helps to illuminate interactions that may not be obvious and allows for experimentation designed to gain insight into what is observed in the field. I*n*HM has been successfully employed at the catchment scale (VanderKwaak and Loague, 2001; Loague and VanderKwaak, 2002; Loague *et al*., 2004) and is currently being tested at larger scales. Constraining the initial applications of I*n*HM to *real* problems establishes the necessary foundation for the ongoing concept-development simulations of hypothetical realities.

One major advantage that I*n*HM has over most hydrologic response models is the ability to simulate solute transport (see Table I). Tracer experiments, of the type reported by Anderson *et al.* (1997) and McDonnell (1990), can further help to test physics-based models. For example, if the transport of a tracer is simulated incorrectly, then the representativeness of the simulated flow (which drives the transport) should be questioned. An ongoing justification for developing, using, and revising tools like I*n*HM is to advance (with minimal presumption) our understanding of the non-intuitive interplay between processes that are not mutually exclusive (e.g. Horton and Dunne overland flow).

> Data, Data, Data! He cried impatiently. I can't make bricks without clay.
>
> Sherlock Holmes

But There Are (Of Course) Problems

The structure of a physics-based model and the characterization/parameterization of a BVP is an iterative process. In our opinion, this approach has not yet been exhausted for models like I*n*HM. For example, if using Richards' equation to describe flow in macropores (i.e. the dual continuum approach employed by I*n*HM) is shown to be incorrect, then it should (and can) be replaced, once the correct physics is known. The data requirements for rigorous physics-based catchment-scale simulations of near-surface hydrologic response are significant (and unlikely to be routinely met anytime soon), but they are not a reason, despite seemingly slow progress, to give up (i.e. we have been to the Moon and back and landed on Mars).

There are many problems associated with the characterization and parameterization of a given

Table II. Comparison of two steady-state infiltration measurements made at the same location

Measurement date, air temperature	Saturated hydraulic conductivity estimate		Permeability estimate[a]	
	K_s (m s^{-1})[b]	Difference (%)[c]	k (m^2)[d]	Difference (%)
5 October 1984, 30 °C[e]	2.87×10^{-5}		2.35×10^{-12}	
9 November 1984, 26 °C[f]	3.2×10^{-6}	797	2.8×10^{-13}	739

[a] $k = K_s\mu/\rho g$, where ρ is fluid density [ML^{-3}], g is acceleration due to gravity [LT^{-2}], and μ is dynamic fluid viscosity [$ML^{-1}T^{-1}$].
[b] See Loague and Gander (1990).
[c] Difference (%) = [(Larger value − Smaller value)/Smaller value] ×100.
[d] See Loague and Kyriakidis (1997).
[e] Measurement located on transect #1 (see Loague and Gander (1990: figure 1)).
[f] Measurement located on transect #2 (see Loague and Gander (1990: figure 1)).

BVP for distributed hydrologic modelling (e.g., Beven, 1989, 1993, 1996a,b, 2000a,b, 2001b,c, 2002a,b; Beven and Binley, 1992; Woolhiser, 1996; Beven and Freer, 2001; Singh and Woolhiser, 2002). One of the bigger, yet often ignored, obstacles in effectively exciting a physics-based model is the assumption of time invariance for system parameters. For example, Table II shows saturated hydraulic conductivity and permeability estimates for a single location where the steady-state infiltration measurement was repeated (i.e. intersection of two transects). The time between the two measurements was a relatively short 35 days. However, the saturated hydraulic conductivity and the permeability both differ, by 797% and 739% respectively, between their initial and final estimates. It is clear that, for these two measurements, the temperature-related (i.e. density and viscosity) differences for the estimates of saturated hydraulic conductivity are smaller than the differences related to changes in permeability. Obviously, for this measurement pair, the permeability estimates are not time invariant. The worst way to interpret this problem is that two data points are not always better than one. Without time invariance for near-surface soil hydraulic parameters, the *space–time tradeoff* concept, defined as an increase in model efficiency achieved through a one-time increase in measurement points as opposed to a lengthening of records, cannot be the linch-pin between data-worth considerations and rigorous evaluation of underlying modelling techniques as proposed by Freeze (1982) and Loague (1991). Obviously, the time-invariance problem does not only plague deterministic-conceptual models.

The various calls for detailed long-duration field monitoring programmes at selected experimental catchments (e.g. Dunne, 1983, 1998; Entekhabi *et al.*, 1999), in the spirit of the *International Hydrologic Decade*, are renewed here. For example, surface soil-water content data, whether acquired via advanced technology or by the *squish test*, is needed for critical evaluation of the response of even the simplest hydrologic system. It should also be mentioned that there are no established model performance standards for different applications.

> I'm older now but still runnin' against the wind
>
> Bob Seger

The Bottom Line

The measure and model approach, pioneered by Horton (see Beven (2004b)), is without question the best protocol in hydrology. For example, without the detailed field experiments of Dunne and Black (1970a,b) and the process-based simulations of Freeze (1971, 1972a,b), the chronology of advances in hillslope hydrology would almost certainly have been different. In the 1970s, physics-based hydrologic-response simulation was limited by both computer speed/storage and field data. For example, the simulations by Freeze (1972a,b) and

Stephenson and Freeze (1974), despite the capability of the model, were, in part due to computer resources, 2D vertical slices that did not represent the importance of lateral inflows related to convergence. Today, with on-demand computing facilitated by new technologies such as the GRID (Beven, 2003), computers are no longer the Achilles heel. Data shortfalls, however, persist as a major problem for physics-based simulation. It is important to recognize that heuristic simulation can have great utility when developing the conceptual understanding of hydrologic response needed for designing the next experiment or data collection campaign. Again, it is our contention that the Freeze and Harlan blueprint has not been fully tested and, therefore, should not be rejected.

One of the six myths that Bras *et al.* (2003) discuss, relative to mathematical modelling (in geomorphology), is that *behind every good model there is a solution to partial differential equations*. Obviously, depending upon the application, not every hydrologic-response model needs to fit into Clarke's deterministic-conceptual classification. However, the quest for a physics-based model is not a ridiculous effort, equivalent to Ettinger's (1965) platinum bridge (i.e. an expensive endeavour with little practical utility). It also seems only fair (especially for those old enough to remember the story of the 1958 Edsel; Bonsall, 2002) that physics-based simulation should not be dismissed just because not everyone is a fan. It is our opinion that there is still great utility for physics-based simulation of near-surface hydrologic response. Deterministic-conceptual simulation can facilitate (i) concept development, (ii) hypothesis testing, (iii) evaluation of existing (and future) data sets, (iv) design of field experiments, (v) creation of synthetic data sets, (vi) hosting Monte Carlo experiments, (vii) driving physics-based solute transport and landscape evolution models, and (viii) the development and testing of simpler models.

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